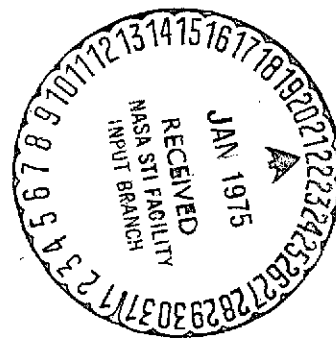


HEAT ESCAPE AND DIFFUSION OF HYDROGEN AND DEUTERIUM
IN THE THERMOSPHERE OF THE EARTH

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ANNOTATION

The problem of escape and diffusion of hydrogen and deuterium atoms from the thermosphere of the Earth is solved by the Monte Carlo method for the model of a stationary, flat atmosphere. The concentration profiles which are obtained are compared with a numerical solution of the diffusion equation. The question of the violation of the Maxwell velocity distribution of H atoms is analyzed, and the effect of this violation on the magnitude of the escape flux and concentration profiles is considered.

HEAT ESCAPE AND DIFFUSION OF HYDROGEN AND DEUTERIUM IN THE THERMOSPHERE OF THE EARTH

Yu. G. Malama

Introduction

The phenomenon of escape of light atoms from the gravitational field of a planet and the diffusion flux which arises as a result determine to a large extent the concentration profile of these atoms in the thermosphere and exosphere. The usual method for the theoretical determination of concentration profiles of small components consists of formulating a model of the atmosphere with subsequent solution of the diffusion equation [1, 2], which, taking turbulence into account, has the form: /3*

$$S_e = -D_1 \left[\frac{dn_1}{dz} + \frac{n_1}{H_1} + (1+d_1) \frac{n_1}{T} \frac{dT}{dz} \right] - D_t \left[\frac{dn_1}{dz} + \frac{n_1}{H} + \frac{n_1}{T} \frac{dT}{dz} \right] \quad (1)$$

Here, n_1 , D_1 , d_1 , S_e are, respectively, the concentration, coefficients of diffusion and thermal diffusion, and escape flux of atoms of the small component in the atmosphere; D_t is the turbulent diffusion coefficient; T is the temperature of the atmosphere; $H_1 = kT/m_1 g$ and $H = kT/mg$ are the altitude scales of the small component

* Numbers in the margin indicate pagination in the original foreign text.

and the atmosphere, respectively; g is the acceleration of gravity; m_1 is the mass of atoms of the small component; \bar{m} is the average mass of the atmospheric particles. The well known Jeans [3] formula is usually used for the flux S_e :

$$\left. \begin{aligned} S_e^{(0)} &= n_1(z_c) \cdot w_e^{(0)}(z_c), \\ w_e^{(0)}(z) &= \left[\frac{g(z) \cdot H_1(z)}{2\pi} \right]^{1/2} \cdot \left[1 + \frac{z}{H_1(z)} \right] \exp \left[-\frac{z}{H_1(z)} \right], \end{aligned} \right\} \quad (2)$$

where z_c is the critical level, defined from the condition:

$$\bar{H} \cdot N\sigma = 1, \quad (3)$$

and $N\sigma$ is the macroscopic cross section for an atom of the small component colliding with particles of the atmosphere.

At altitudes up to $Z \sim (200 - 300)$ km, where the effective Knudsen numbers $K = \lambda/H \ll 1$ (λ is the mean free path), Equation (1) /4 is undoubtedly valid. However, with the approach to $Z = z_c$, where by definition $K = 1$, we are in principle outside the region of applicability of the hydrodynamic description [4], and thus it is difficult to obtain an estimate, within the framework of hydrodynamics, of the error which arises in the use of Equation (1).

The Jeans formula (2) comes in for criticism also. Two assumptions underlie the derivation of this formula: (1) for all $Z < z_c$, the Maxwell velocity distribution is preserved for atoms of the small component, and (2) atoms with velocities satisfying the escape condition experience no collisions above a critical level. It is evident that use of these assumptions must lead to an overestimate of the escape flux.

These difficulties may be overcome by solving the problem of escape and diffusion of light atoms of the small component with the help of the Monte-Carlo method [5 - 12], which enables one to find a physically precise solution for all Knudsen numbers and for any deviations from the Maxwell-Boltzmann distribution.

Kastner [5] studied the diffusion of H atoms in an atmosphere of N_2 with barometric altitude distribution, without taking into account the effect of gravity on the motion of the H atoms. From his results, it follows, in particular, that already for $K \approx 0.003$, the effective diffusion coefficient is about two times less than the value which follows from kinetic theory; however, the methodological errors tolerated in [5] makes this conclusion, which is so radical for hydrodynamics, doubtful.

In [6 - 10], fundamental attention was given to obtaining a correction to the Jeans formula (2). Of these works, only [9, 10] obtained values of the escape flux which were close to each other. The discussions in [9, 13, and 14] on the cause of the discrepancies did not lead to any definite conclusions. The required clarity was supplied by Brinkmann [10], who pointed out errors allowed by the authors of [5 - 7, 9] in generating certain random quantities. /5

At the same time, while there are no theoretical objections to the purely Monte Carlo procedures used in [10] and subsequently in [11, 12], there are, in our view, well known objections to the physical formulation of the problem in these works. In fact, the atmosphere in [10 - 12] was approximated by a uniform layer of O gas atoms. In reply to a remark by Liwshitz and Singer [7] on the unreality of the model, Brinkmann [10] has pointed out that the degree of violation of the Maxwell velocity distribution for H atoms is defined by the "optical" thickness of the layer, calculated from its upper boundary, and, as a consequence of this, the models of the atmosphere with uniform and barometric distributions of the fundamental gas are physically equivalent. If one views the goal of the Monte Carlo calculations as being only to obtain a correction to the Jeans formula (2), then the point of view of the authors of [10 - 12] is justified. However, as was indicated above, a check of the applicability of the diffusion equation (1) is of significant interest, and in this case the nonuniformity of the atmosphere plays a decisive role.

Thus, the formulation of the Monte Carlo part of the problem must be, in our opinion, broader than in [10 - 12], and should be as follows: it is necessary to calculate the escape flux and concentration profile for the atoms which are of interest to us, i.e., the atoms of the small component in the region $Z_{\min} \leq Z \leq Z_{\max}$, and it is desirable that the temperature and concentration profiles of the fundamental components of the atmosphere correspond sufficiently closely to reality. Concerning the choice of boundaries for the layer of atmosphere, one can say the following. Since with a decrease of Z_{\min} , the number of collisions experienced by an atom and, thus, the calculation time rapidly increase (in a number of variations, it increases exponentially), there is no advantage to placing Z_{\min} at the base of the thermosphere. At the same time, the values of Z_{\min} and Z_{\max} must be such that the hydrodynamic and free-molecule approximations in the regions $Z \lesssim Z_{\min}$ and $Z \gtrsim Z_{\max}$, respectively, are undoubtedly applicable. In addition, it is necessary to choose a sufficiently large optical thickness of the layer of atmosphere, such that in the region immediately above Z_{\min} the Maxwell velocity distribution is preserved for atoms of the small component. /6

Statement of the Problem

The main goal of the present paper is to check the applicability of the hydrodynamic solution of the problem of escape and diffusion of H and D atoms in the upper atmosphere of the Earth. Since, as in the preceding papers, a stationary one-dimensional model of the atmosphere is used, the numerical results presented below differ from observational data obtained, for example, by measurements of the Lyman- α line absorption.

It is assumed that below 90 km, turbulent diffusion leads to complete mixing of the components of the atmosphere, and that above 90 km, there are no sources of H and D atoms. The temperature of the atmosphere was considered constant for $90 \text{ km} \leq Z \leq 120 \text{ km}$.

For the region $Z > 120$ km, the model of [15] was used:

$$T(Z) = T_{\infty} \left[1 - \frac{T_{\infty} - T(Z_0)}{T_{\infty}} \exp(-\tau) \right], \quad (4)$$

$$\tau = [T_{\infty} - T(Z_0)]^{-1} \left(\frac{dT}{dZ} \right)_{Z=Z_0} \xi, \quad \xi = \int_{Z_0}^Z \frac{g(Z')}{g(Z_0)} dZ',$$

where $Z_0 = 120$ km, T_{∞} is the model parameter, $T(Z_0) = 355^{\circ}$ K, /7
 $(dT/dZ)_{Z=Z_0} = 20$ deg/km. The model atmosphere consists of O, O₂, N₂, and Ar, with concentrations at altitude $Z = 120$ km, $n(O) = 9.6 \cdot 10^{10}/\text{cm}^3$, $n(O_2) = 6.0 \cdot 10^{10}/\text{cm}^3$, $n(N_2) = 4.5 \cdot 10^{11}/\text{cm}^3$, and $n(\text{Ar}) = 2.2 \cdot 10^9/\text{cm}^3$ [16]. For the remaining altitudes $Z \geq 90$ km, the concentrations of the fundamental components were found by integration of Equation (1) with $S_e = 0$.

The trajectories of the H and D atoms were simulated by the Monte Carlo method in the region $250 \text{ km} < Z < 1000 \text{ km}$ [it was considered that for $90 \text{ km} < Z < 250 \text{ km}$ the diffusion equation (1) is valid]. In this region, only O atoms and N₂ molecules are taken into account (in some calculations He atoms were also added, but the results with these atoms were practically unchanged). As it is subsequently proposed to combine the Monte Carlo results with the solution of Equation (1), it was considered to be expedient to take into account the direct effect of the force of gravity on the motion of H and D atoms, in contrast to the previous papers.

The entire region (Z_{\min}, Z_{\max}) was divided into 30 layers, within each of which the acceleration of gravity, the temperature, and the concentrations of all components of the atmosphere were considered constant. The collisions were assumed to be purely elastic; for deuterium a solid sphere model was used, while in the case of hydrogen, two series of calculations were carried out — one with a solid sphere cross section, and one with a cross section found beforehand by the WKB method [17]. In the first case, the numerical values were:

$$\sigma_{H-O}^{(t)} = 1.713 \cdot 10^{-15} \text{ cm}^2 \text{ and } \sigma_{H-N_2}^{(t)} = 3.285 \cdot 10^{-15} \text{ cm}^2,$$

and in the second, the only difference from [10] was a modification of the interaction potential with account of the four electronic states of $O(3p) - H(2s)$ system [18, 19]. In particular, for the average total $O + H$ collision cross section, the approximation: /8

$$\sigma_{H+O}^{(t)} = \begin{cases} 3.36 \cdot 10^{-14} \text{ cm}^2, & u \leq 0.2v_0 \\ 10^{-15} (3.04 + 1.56 \frac{v_0}{u} + 0.91 \frac{v_0^2}{u^2}) \text{ cm}^2, & u > 0.2v_0 \end{cases} \quad (5)$$

was obtained, where u is the speed of relative motion, and $v_0 = 4.08 \cdot 10^5$ cm/sec is the thermal speed of H atoms at $T = 10^3$ K.

Let us now consider the choice of the calculational scheme. Brinkmann [10] has shown that for small values of the parameter $mv_e^2/2kT$, where v_e is the minimum escape velocity, the application of direct Monte Carlo simulation for the calculation of the escape flux is not effective. Instead of this, he proposed the method of "mirror" particles, which is in essence a particular case of the method of separating out the principal part [20]. The latter is based on representing the required solution in the form of a sum of two terms $f = f_1 + f_2$, where it is assumed that one of them, let us say f_1 , is either known beforehand or can be easily found by other methods. If, furthermore, the correction f_2 can be found by the Monte Carlo method, then the problem as a whole is thereby solved. The effectiveness of the method of separating out the principal part increases with increasing strength of the inequality $|f_1| > |f_2|$.

In the problem being considered, it is natural to choose as the known function not the uniform distribution, as in [10], but the solution of the generalized barometric equation:

$$\frac{d\tilde{n}_2}{dz} + \frac{n_1}{H_1} + (1+\alpha_1) \frac{n_1}{r} \frac{dT}{dz} = 0, \quad (6)$$

which we denote by $n_1^{(0)}(Z)$. The actual solution is then equal to: /9

$$n_1(Z) = n_1^{(0)}(Z) - n_1^{(-)}(Z), \quad (7)$$

where the function $n_1^{(-)}(Z)$, as in [10], is the concentration profile for atoms of the small component with a source in the plane $Z = Z_{\max}$. The strength of this source is equal to:

$$S^{(-)} = n_1^{(0)}(Z_{\max}) \cdot w_e^{(0)}(Z_{\max})_2 \quad (8)$$

where $w_e^{(0)}$ is defined by Relation (2).

Description of the Computational Methods

The position of an atom in phase space is characterized by the coordinate Z and by the velocity components v_x, v_y, v_z (the introduction of three components instead of two is purely for calculational convenience). The sequence of a simulation of trajectories of atoms contributing to the profile $n_1^{(-)}$ is given below (more cumbersome algorithms are presented in the appendix).

1. Injection of atoms into a layer of atmosphere in the plane $Z = Z_{\max}$. For the velocity vector

$$\vec{V} = \{v \sin \theta \cos \varphi, v \sin \theta \sin \varphi, v \cos \theta\},$$

we have a distribution density which is proportional to the flux:

$$P(v, \theta, \varphi) dv d\theta d\varphi = \begin{cases} 0, & v < v_e \\ A v^3 e^{-\frac{mv^2}{2kT}} dv \sin \theta \cos \theta d\theta d\varphi, & v \geq v_e \end{cases} \quad (9)$$

where A is the normalization constant, and the values v_e and T refer to the plane $Z = Z_{\max}$. The value of $\cos \theta$ is generated according to* $\cos \theta = -\sqrt{\beta}$, while the values of $\cos \phi, \sin \phi$ are generated

*Here and below, β is a running random number, uniformly distributed in the interval $(0, 1)$.

by the Neumann method [20]:

$$\left. \begin{aligned} \cos \varphi &= \frac{\xi_1}{\sqrt{\xi_1^2 + \xi_2^2}}, \quad \sin \varphi = \frac{\xi_2}{\sqrt{\xi_1^2 + \xi_2^2}}, \\ \xi_1 &= 1 - 2\beta_i \end{aligned} \right\} \quad (10)$$

with rejection for $\xi_1^2 + \xi_2^2 > 1$. The quantity v was generated in accordance with Expressions (A-1) and (A-2). /10

2. Simulation of the trajectory of an atom in the i^{th} layer ($Z_i < Z < Z_{i+1}$). In the general case, an atom can either experience a collision with one of the particles of the atmosphere, or leave this layer without collisions. The macroscopic cross section for collision of an atom with particles of the atmosphere is equal to:

$$\sigma_m(v) = \sum_{\alpha} \langle \sigma_{\alpha}^{(t)} \rangle \cdot n_{\alpha, i}, \quad (11)$$

where $n_{\alpha, i}$ is the concentration of the α^{th} component in the layer i , and $\langle \sigma_{\alpha}^{(t)} \rangle$ is the mean integral collision cross section for an atom with a particle of type α . This cross section has the form [10]:

$$\langle \sigma_{\alpha}^{(t)} \rangle = \frac{2\pi}{v^2} \left(\frac{m_{\alpha}}{2\pi k T_i} \right)^{3/2} \int_0^{\infty} v_{\alpha} e^{-\frac{m_{\alpha} v_{\alpha}^2}{2k T_i}} dv_{\alpha} \cdot \int_{|v-v_{\alpha}|}^{v+v_{\alpha}} u^2 \sigma_{\alpha}^{(t)}(u) du \quad (12)$$

Using the notation $\kappa^2 = \frac{m_{\alpha} v^2}{2k T_i}$, $x^2 = \frac{m_{\alpha} v_{\alpha}^2}{2k T_i}$, $y^2 = \frac{m_{\alpha} u^2}{2k T_i}$, it is convenient to write the latter expression in the form:

$$\langle \sigma_{\alpha}^{(t)} \rangle = \frac{2}{\sqrt{\pi}} \cdot \frac{1}{\kappa^2} \int_0^{\infty} x e^{-x^2} dx \int_{|x-x|}^{\kappa+x} y^2 \sigma_{\alpha}^{(t)}(y) dy \quad (13)$$

The values of $\langle \sigma_{\alpha}^{(t)} \rangle$ were calculated beforehand for 48 discrete values of K in the interval $(0, 20)$, on the basis of which the values of $\langle \sigma_{\alpha}^{(t)} \rangle(v)$ and $\sigma_m(v)$ were found by linear interpolation. After establishing the mean free path of an atom:

$$t_c = -[\nu \sigma_m]^{-1} \ln \beta \quad (14)$$

the time t_i of its collisionless existence in the i^{th} layer was calculated (taking into account the force of gravity). For $t_i \leq t_c$, it was considered that the atom had left this layer without collision, and it was given new coordinates: /11

$$Z' = \begin{cases} Z_i, & v_z \leq 2g_i(Z_{i+1} - Z) \\ Z_{i+1}, & v_z > 2g_i(Z_{i+1} - Z) \end{cases} \quad (15)$$

and components v_Z :

$$v_z' = v_z - g_i t_i \quad (16)$$

In the opposite case $t_i > t_c$, the values of Z and v_Z were also calculated, and it was considered that a collision had taken place.

3. Generation of the collision. In the first stage, a selection of the particle partner type was made with respect to the collision; the corresponding probabilities follow directly from (11). For the parameters of this particle, we have the distribution density:

$$p(v_\alpha, \cos \alpha; v) = A u G_\alpha^{(t)}(u) v_\alpha^2 \exp\left(-\frac{m_\alpha v_\alpha^2}{2kT_i}\right), \quad (17)$$

where A is an insignificant normalization constant. The algorithm for generating the quantities v_α and $\cos \alpha$ is presented in the appendix [Formulas (A-3) - (A-7)]. Although the formulas for calculating the results of the collision itself are simple, they are somewhat cumbersome, and will not be presented here.

Steps 1 - 3, in fact, exhaust the algorithms for simulation of the trajectories. The boundary conditions, analogously to [10], are reduced to a cutoff of the trajectories either for $Z = Z_{\min}$, or for simultaneous fulfillment of the conditions $Z = Z_{\max}$, $v \geq v_e$. For $Z = Z_{\max}$, $v < v_e$, a mirror reflection of the particle is carried out: $v_Z' = -v_Z$.

The quantities $\Sigma\tau_i$ and $\Sigma\tau_{ip}$ were calculated for N statistically independent trajectories, where τ_i is the time spent by an atom in the i^{th} layer, τ_{ip} is the time spent by an atom in the phase cell (Z_i, v_p) with volume $\Delta Z \cdot \Delta v$, and the summation is carried out over all the trajectories. In addition, the number of escaping atoms $N^{(-)}$ was calculated. After realization of all N trajectories, the concentration:

$$n_i^{(-)}(z) = (\Delta z)^{-1} \sum \tau_i \quad (18)$$

was found for each layer (the velocity distribution functions were determined similarly). Finally, the concentration profile:

$$n_z(z) = n_z^{(0)}(z) - \frac{n_1^{(0)}(z_{\max}) \cdot w_e^{(0)}(z_{\max}) \cdot n_1^{(-)}(z)}{N} \quad (19)$$

and escape flux:

$$S_e = n_1(z_e) \cdot w_e(z_e) = n_1^{(0)}(z_{\max}) \cdot w_e^{(0)}(z_{\max}) \left[1 - \frac{N^{(-)}}{N} \right] \quad (20)$$

were calculated in accordance with Expressions (7) and (8).

The escape flux found by the Monte-Carlo method was substituted into the diffusion equation (1), which was then numerically integrated from $Z = 90$ km to $Z = 800$ km, with normalization $n_H(90 \text{ km}) = 1$, $n_D(90 \text{ km}) = 1.5 \cdot 10^{-4}$. For the coefficients D_1 and α_1 , the values corresponding to the solid sphere model [17] were used:

$$\left. \begin{aligned} D_1 &= 0.212 \sqrt{r} \left(\frac{2\kappa T}{m_1} \right)^{1/2} \left[\sum \left(\frac{\mu_{1d}}{1 + \mu_{1d}} \right)^{1/2} n_d \sigma_d^{(e)} \right]^{-1} \\ \alpha_1 &= -0.385 \end{aligned} \right\} \quad (21)$$

where the summation is carried out over all fundamental components of the atmosphere, $\mu_{1d} = \frac{m_d}{m_1}$, and the turbulent diffusion coefficient

was set equal to the constant value $D_t = 5 \cdot 10^6$ cm/sec, recommended in [21]. The concentration profiles calculated by the Monte Carlo

method were then joined with the solution of Equation (1) in the region $Z \gtrsim 250$ km.

Results of the Calculations

Let us first of all consider results of calculations for the diffusion of atoms in a flat isothermal atmosphere' composed of a single type of particle with an exponential distribution of concentration along the Z axis. As in [5], the force of gravity is not taken into account here. Substituting the values of the flux S and the concentration profiles $n_1(Z)$ of the small component obtained by the Monte Carlo method into the formal diffusion equation: /13

$$S = -D \frac{dn_1}{dz} \quad (22)$$

it is possible to calculate the values of the effective diffusion coefficient D for different Knudsen numbers (Figure 1). It is seen that the deviation of D from the value D_g , which follows from kinetic theory [17], is about 10% for $K = 0.4$, and about 35% for $K = 10$.

Let us now discuss results obtained in the solution of the problem of the escape and diffusion of H and D atoms. Several calculations were carried out for both of these small components with a solid sphere model for five values of the exosphere temperature (750, 1000, 1250, 1500, and 2000° K). In the case of hydrogen, similar calculations were done with cross sections obtained by the WKB method. In addition, for $T_\infty = 1500^\circ$ K, a calculation was carried out by the direct Monte Carlo simulation method. The results of the simulation agreed with the results obtained by the method of separating out the principal part, to within the limits of statistical error.

Figure 2 shows "mirror" and real profiles of effective temperatures for H atoms (solid sphere model) for three values of T_∞ . The mirror profiles can serve as a very sensitive criterion for the correctness of the choice of optical thickness for the layer of

atmosphere. It is seen that the maxwellization of the mirror atoms is totally completed in a distance of about 20λ from Z_{\max} . Thus, the choice of a layer of atmosphere with thickness less than 20λ can lead to physically incorrect results. In connection with this, it can be noted that in the work of Brinkmann [10], the tendency toward increase of the escape flux with a decrease of the layer thickness from 15λ to 10λ , and further to 5λ is clearly traced. Such a significant optical thickness for the layer $Z_{\max} - Z_{\min} = 20 \lambda$, which is necessary for preserving the Maxwell distribution of H atoms near Z_{\min} , is explained, of course, by the low effectiveness [in the] transmission of energy during collisions of particles with very different masses.

Figure 3 shows the corrections to the Jeans magnitude $S_e^{(0)}$ for the escape flux which were obtained with the Monte Carlo method in comparison with the data of [10, 11]. The completely satisfactory agreement is explained, apparently, by the fact that the degree of violation of the Maxwell distribution of H atoms at the altitude Z depends only on the optical thickness $(Z_{\max} - Z)/\lambda$, and on the mass ratio for the atoms of the small component and the fundamental gas of the atmosphere. The nonuniformity in the concentration of the atmosphere does not affect these results. We also confirmed the conclusion by the authors of [10, 11] that the inaccuracy in determining the collision cross section is weakly manifested in the magnitude of the ratio $S_e/S_e^{(0)}$. The presence of a weak minimum at $T_{\infty} \sim 1250^\circ \text{ K}$ follows from our data. Although this minimum might be completely explained by statistical error, its appearance is not physically meaningless. In this connection, one can, apparently, make an analogy with the violation of the Maxwell velocity distribution in chemically reacting gases. Analytic calculations using the generalized Chapman-Enskog method and Monte Carlo calculations [22] have distinctly shown the presence of a minimum in the temperature dependence of the ratio $R/R^{(0)}$, where R is the true reaction rate,

and $R^{(0)}$ is the reaction rate with the assumption that the Maxwell velocity distribution is preserved for the reacting particles.

Figure 4 shows concentration profiles for H atoms (solid sphere model) for three values of T_∞ . At low temperatures (curve 1), the profiles calculated by the Monte Carlo method and those obtained by direct integration of Equation (1) coincide in practically the whole region $250 \text{ km} < Z < 800 \text{ km}$. This result is explained by the fact that, for a small escape flux, the concentration profile for H atoms is practically the same as the generalized barometric distribution, which, as is well known, is valid for any Knudsen numbers.

A first glance, the concentration profiles at higher temperatures appear strange: in the first place, one might expect that the deviation of the Monte-Carlo profiles from the solution of Equation (1) must increase with an increase of T_∞ . Secondly, another sign for these deviations seems to follow from the results presented in Figure 1. In fact, since the Monte Carlo values of the escape fluxes S_e were used in the integration of (1), a decrease of the effective diffusion coefficient with an increase of K should lead, despite Figure 4, to more strongly negative gradients of the Monte Carlo concentration profile in comparison with the hydrodynamic profile.

The indicated contradictions can, however, be explained by analyzing Equation (1). Since for $Z > 250 \text{ km}$, the turbulent diffusion process plays no role, this equation can be written in the form: /16

$$-\frac{dn}{dz} = \frac{n}{H} + \frac{S_e}{D} + (1+\alpha) \frac{n}{T} \frac{dT}{dz} \quad (23)$$

For $Z \geq 400 \text{ km}$, the third term on the right hand side of (23), describing the process of thermal diffusion, is negligible, because the atmosphere at such high altitudes is isothermal. However, Equation (23) does not take into account the fact that the escape of fast atoms with $v \geq v_e$ leads to a violation of the Maxwell velocity distribution for H atoms, as a consequence of which a negative gradient of the effective temperature of these atoms is established

at altitudes $Z \geq 400$ km (Figure 2). As a result, a thermal diffusion flux must arise from bottom to top, tending to level out the negative gradient in the concentration of H atoms. Thus, the magnitude and sign of the total Monte Carlo correction to the solution of Equation (23) depend both on the ratio of the separate corrections to the flux and thermal diffusion terms on the right side of this equation, and on the absolute values of these terms. At low atmospheric temperatures, the quantity S_e is also small; as a consequence, one might expect fulfillment of the inequality:

$$\frac{S_e}{D_1} < (1 + \alpha_1) \frac{n_1}{T} \left| \frac{dT}{dz} \right|,$$

which explains the sign of the Monte Carlo correction for $T_\infty = 1500^\circ$ K. However, as the atmospheric temperature increases, so does the importance of the term S_e/D_1 . Evidently, it is precisely this which explains the lesser values of the corrections for $T_\infty = 2000^\circ$ K, in comparison with the case, $T_\infty = 1500^\circ$ K.

Profiles of the ratio of the deuterium concentration to the hydrogen concentration for various values of T_∞ are shown on Figure 5. The increase in the values of n_D/n_H with the increase of T_∞ from 750 to 1250° K, and the decrease of these values upon further increase of T_∞ to 2000° K, are in good agreement with the conclusions of McElroy and Hunten [2]. The presence of maxima on the profiles for all T_∞ , excluding the value 2000° K, is in qualitative agreement with the data of measurements of Lyman- α line absorption [23], and is explained, apparently, by the effect of separation by diffusion of isotopes at high altitudes. The absolute values of the quantity n_D/n_H for $T_\infty = 1200^\circ$ K presented in [23] are approximately an order of magnitude larger than in the present paper. The cause of such significant discrepancies might be, first, that the data of [23] are not the result of direct observations (they are obtained, as the authors note, as the result of the introduction of several assumptions). In connection with this, it may be noted that the results of spectroscopic measurements of the concentration of D^+ ions at altitudes of (500 - 3000) km give values close to the concentrations

/17

of H^+ ions [24]. On the other hand, the one-dimensional, flat model of the atmosphere used in our calculations is a crude approximation, and this could strongly distort the results.

It seems to us that for development of this work, it is necessary to give up the flat model of the atmosphere in the Monte Carlo calculations, and to take into account, in addition, the diurnal variations in the temperature and concentrations of the fundamental components of the atmosphere. It is also evident that the method described could be extended without difficulty to such planets as Venus and Mars.

The complexity of the structure of planetary atmospheres and the multitude of physical and chemical processes which occur in these atmospheres make the use of analytic and traditional numerical methods extremely difficult. It is also impossible to disregard the violations of thermodynamic equilibrium which take place. In many cases, these violations can significantly limit the region of applicability of these methods, which are based on a macroscopic description. For these reasons, the use of Monte Carlo simulation is extremely promising. Besides mathematical simplicity and suitability for computer use, this method also has theoretical advantages. The primary advantage is its indifference to the degree of violation of thermodynamic equilibrium and to the values of the Knudsen number. /18

The author is grateful to V. B. Leonas for attention to the work and for useful advice.

APPENDIX

Although all of the algorithms presented by Brinkmann [10] for /19
the simulation of random quantities are correct, some of these algorithms are not completely appropriate. The method of integral probability, which is universally used by Brinkmann, frequently leads to only an approximate selection of the random quantity with specified distribution law. In addition, in a number of cases (for example, in the generation of the parameters of colliding particles), the application of this method requires large amounts of machine time. In such situations, we have used other effective and accurate methods.

For the random selection of the quantity v for the injected atom, the transformation $x^2 = \frac{m}{2kT}(v^2 - v_0^2)$ was used; this converts the velocity part of Expression (9) into the density:

$$\left. \begin{aligned} \rho_1(x) dx &= \frac{\eta + x^2}{\eta + 1} x e^{-x^2} dx, \quad x \geq 0 \\ \eta &= \frac{mv_0^2}{2kT} \end{aligned} \right\} \quad (\text{A-1})$$

From the form of (A-1), it follows that with probability $(\eta + 1)^{-1/2}$ the quantity x can be considered to be distributed with density $\sim x e^{-x^2}$, and with probability $(\eta + 1)^{-1}$ distributed with a density $\sim x^3 e^{-x^2}$. This is the basis for the choice:

$$x = \begin{cases} [-\ln(\beta_2 \beta_3)]^{1/2}, & (\eta + 1)^{-1} > \beta_1 \\ (-\ln \beta_2)^{1/2}, & (\eta + 1)^{-1} \leq \beta_1 \end{cases} \quad (\text{A-2})$$

The latter expression follows from an exact method of generation an n -dimensional normal law presented in [25].

The Kan* method [26] was taken as the basis of generating the random quantities v_α and $\cos \alpha$, distributed according to the

*Translator's note. Transliterated from the Russian.

density (17). Let us rewrite (17) in the form:

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$$\rho(v_\alpha, \cos \alpha; v) = \frac{Au\sigma_\alpha^{(u)}(u)}{\psi(u)} \left[\psi(u) v_\alpha^2 \exp\left(-\frac{m_\alpha v_\alpha^2}{2\kappa T}\right) \right] \quad (A-3)$$

where the condition $\phi \geq 0$ is imposed on the function ϕ , and $|Au\sigma_\alpha^{(u)} \cdot \psi^{-1}| \leq 1$ for all u , $v_\alpha > 0$, and all values of the quantity v , considered as a parameter. In addition, it is desirable to select ϕ such that $\text{Sup}[Au\sigma_\alpha^{(u)} \psi^{-1}] = 1$. The Kan method consists of generating the quantity v_α according to a density which is proportional to the expression in square brackets in (A-3); the generation of $\cos \alpha$ in the interval $(-1, 1)$, and the calculation of $u = (v^2 + v_\alpha^2 - 2vv_\alpha \cos \alpha)^{1/2}$ and $\sigma_\alpha^{(u)}$. Further, the method of rejection is used: the generated values $v_\alpha \cos \alpha$ are accepted with probability $Au\sigma_\alpha^{(u)} \psi^{-1}$.

The specific choice of the function ϕ depends, naturally, on the form of the cross section $G_\alpha^{(u)}$. Thus, for the solid sphere model, in which the cross section is independent of u , it is natural to put $\psi = (v + v_\alpha) A^{1/2} \sigma_\alpha^{(u)}$. The algorithm for generating the quantities v_α , $\cos \alpha$ was described in [22], and consists of the following:

- a) the quantity v_α is generated according to the rule:

$$v_\alpha = \begin{cases} \left[\varepsilon [-\ln \beta_2 - (\ln \beta_3) \cos^2(\pi \beta_4)] \right]^{1/2}, & v(v + \frac{2}{T} \varepsilon)^{-1} \geq \beta_1 \\ \left[\varepsilon [-\ln(\beta_2 \cdot \beta_3)] \right]^{1/2}, & v(v + \frac{2}{T} \varepsilon)^{-1} < \beta_1 \end{cases} \quad (A-4)$$

$$\varepsilon = (2\kappa T/m_\alpha)^{1/2}$$

- b) $\cos \alpha = 1 - 2\beta_5$ is generated,

- c) the quantity u is calculated; for

$$u(v + v_\alpha)^{-1} \geq \beta_6 \quad (A-5)$$

the generated values of v_α , $\cos \alpha$ are accepted.

In the opposite case, all operations are repeated with new β_1 , beginning with setp a).

In the case of cross section of the form

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$$G_a^{(u)} = \begin{cases} D, & u < u_0 \\ C + \frac{A}{u} + \frac{B}{u^2}, & u \geq u_0 \end{cases} \quad (A-6)$$

the function ϕ is put equal to

$$\psi(u) = C(v + v_0) + A + \frac{B}{u_0} \quad (A-7)$$

The details of the generation of the quantities v_α , $\cos \alpha$ are very similar to steps a) - c), and to save space they will not be presented here.

REFERENCES

1. Bates, D. R. and T. N. L. Patterson. Planet. Space Sci., Vol. 5, 1961, p. 257. /22
2. McElroy, M. R. and D. M. Hunten. J. Geophys. Res., Vol. 74, 1969, p. 1720.
3. Chamberlain, M. W. Planet. Space Sci., Vol. 11, 1963, p. 901.
4. Izakov, M. N. Space Sci. Rev., Vol. 7, 1967, p. 579.
5. Kastner, S. O. J. Geophys. Res., Vol. 69, 1964, p. 157.
6. Lew, S. K. and S. V. Venkateswaran. J. Atm. Sci., Vol. 22, 1965, p. 623.
7. Liwshitz, M. and S. F. Singer. Planet. Space Sci., Vol. 14, 1966, p. 541.
8. Liwshitz, M. J. Geophys. Res., Vol. 72, 1967, p. 285.
9. Chamberlain, J. W. and F. J. Campbell. Astrophys. J., Vol. 149, 1967, p. 687.
10. Brinkmann. Planet. Space Sci., Vol. 18, 1970, p. 449.

11. Chamberlain, J. W. and G. R. Smith. Planet. Space Sci., Vol. 19, 1971, p. 675.
12. Brinkmann, R. T. Planet. Space Sci., Vol. 19, 1971, p. 791.
13. Liwshitz, M. J. Atm. Sci., Vol. 23, 1966, p. 816.
14. Lew, S. K. and S. V. Venkateswaran. J. Atm. Sci., Vol. 23, 1966, p. 817.
15. Bates, D. R. Proceed. Roy. Soc., Vol. A253, 1959, p. 451.
16. Moe, K. J. Geophys. Res., Vol. 78, 1973, p. 1633.
17. Hirschfelder, J., C. Curtiss and R. Byrd. "Molecular Theory of Gases and Liquids". Foreign Literature Publishing House, 1961.
18. Krupenie, P. H., E. R. Mason and J. T. Vanderslice. J. Chem. Phys., Vol. 39, 1963, p. 2399.
19. Solomon, P. M. Nature, Vol. 217, 1968, p. 334.
20. Buslenko, N. P. et al. Metod statisticheskikh ispytaniy (Metod Monte-Karlo) [Method of Statistical Experiments (Monte Carlo Method)]. Fizmatgiz, Moscow, 1962.
21. Hunten, D. M. Comments on Astrophys. Space Phys., Vol. 3, 1971, p. 1.
22. Denisik, S. A., S. N. Lebedev, Yu. G. Malama and A. I. Osipov. Fizika gorennya i vzriva, Vol. 8, 1972, p. 331. /23
23. Jones, R. A., E. C. Bruner and W. A. Rense. J. Geophys. Res., Vol. 75, 1970, p. 1849.
24. Hoffman, J. H. Science, Vol. 155, 1967, p. 322.
25. Marsaglia, G. Ann. Math. Stat., Vol. 32, 1961, p. 899.
26. Sapiier and E. Gelbard. Metod Monte-Karlo i zadachi perenosa neutronov (Monte Carlo Principles and Neutron Transport). Moscow, 1972.

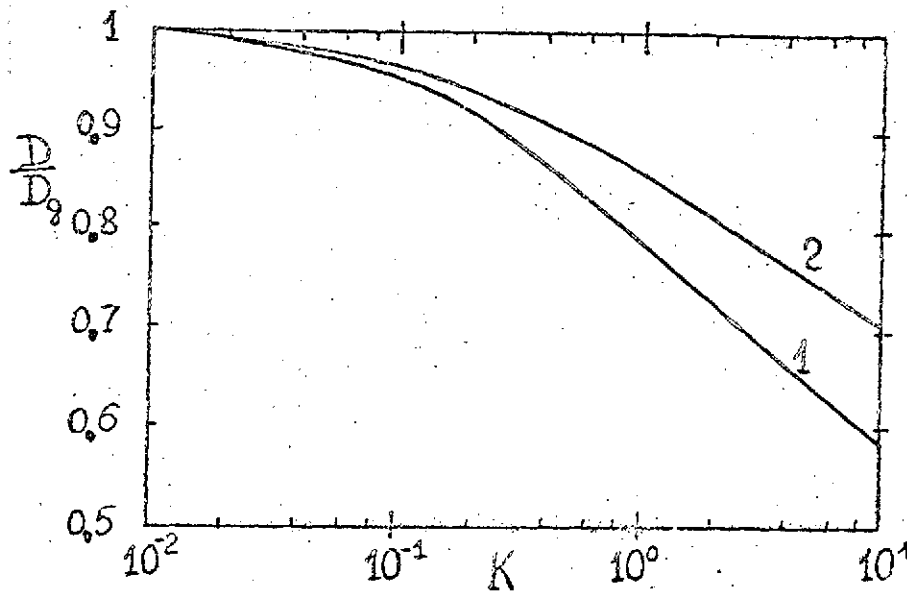


Figure 1. Ratio of effective diffusion coefficient D to the value D_g following from kinetic theory (21), as a function of Knudsen number K :
 1, 2 — diffusion of atoms of mass m_1 in a layer of gas of atoms with mass m_2 for, respectively,
 $m_2/m_1 = 1$, and $m_2/m_1 = 16$

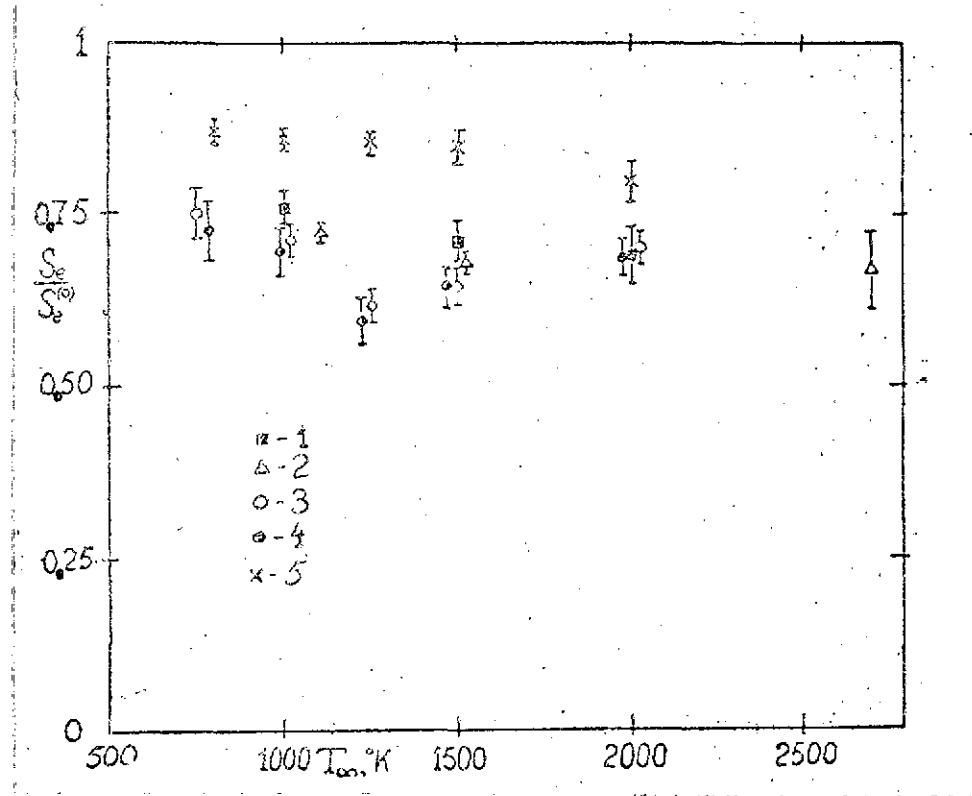


Figure 3. Ratio of the escape flux S_e , found by the Monte Carlo method, to the flux $S_e^{(0)}$ (2) as a function of the temperature of the exosphere T_{∞} :

1 — results of Brinkman [10] for hydrogen (WKB cross section); 2 — results of Chamberlain and Smith [11] for hydrogen (solid sphere cross section); 3, 4, 5 — results of the present paper, respectively, for hydrogen (solid sphere cross section), hydrogen (WKB cross section), and deuterium (solid sphere cross section). The vertical bars are standard deviations

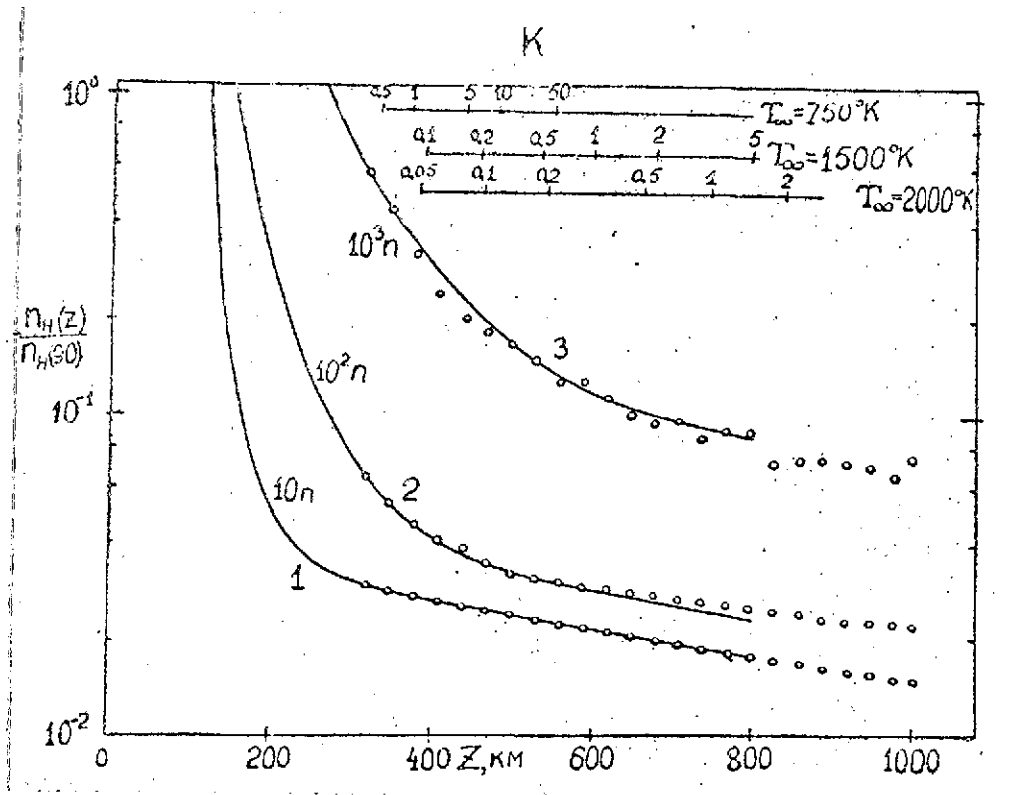


Figure 4. Concentration profiles for H atoms with $T_{\infty} = 750^{\circ} \text{ K}$ (1), $T_{\infty} = 1500^{\circ} \text{ K}$ (2), and $T_{\infty} = 2000^{\circ} \text{ K}$ (3): the curves are the results of a numerical integration of Equation (1); the points are the results obtained by the Monte Carlo method. The upper scale gives Knudsen numbers for various T_{∞}

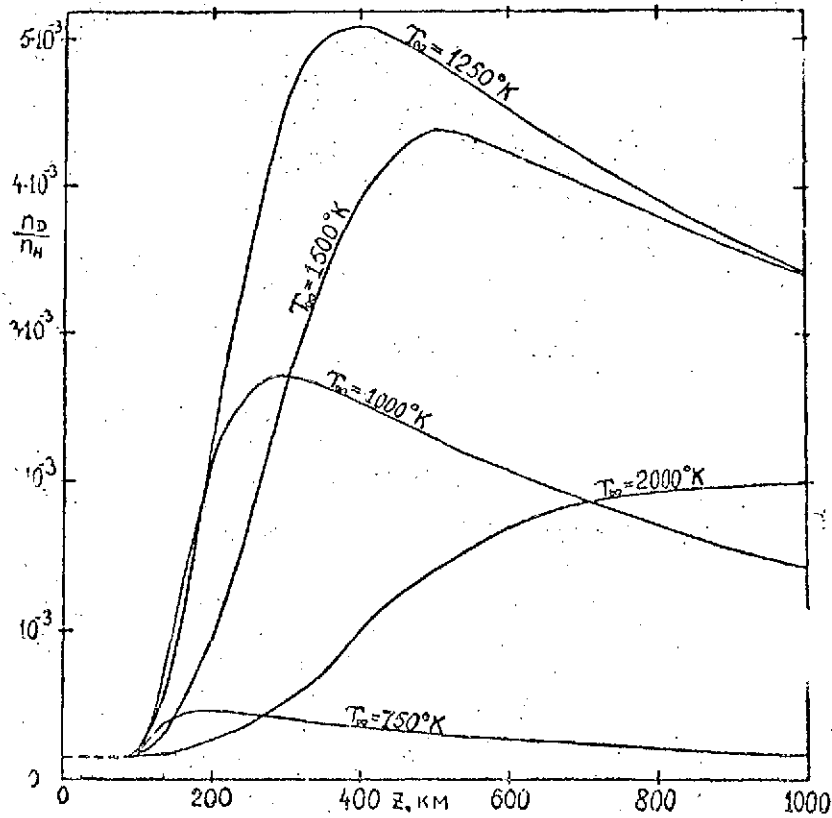


Figure 5. Profiles of the ratio of the concentrations of deuterium and hydrogen for five values of T_{∞} ; the numerical values for $90 \text{ km} \leq Z \leq 250 \text{ km}$ were obtained by solution of Equation (1), while for $250 \text{ km} < Z \leq 1000 \text{ km}$ they were obtained by a Monte Carlo simulation

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